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ON SHAPE NORMALIZATION FOR NON-UNIFORMLY ACTIVE CATALYST PELLET--ETC(U)  
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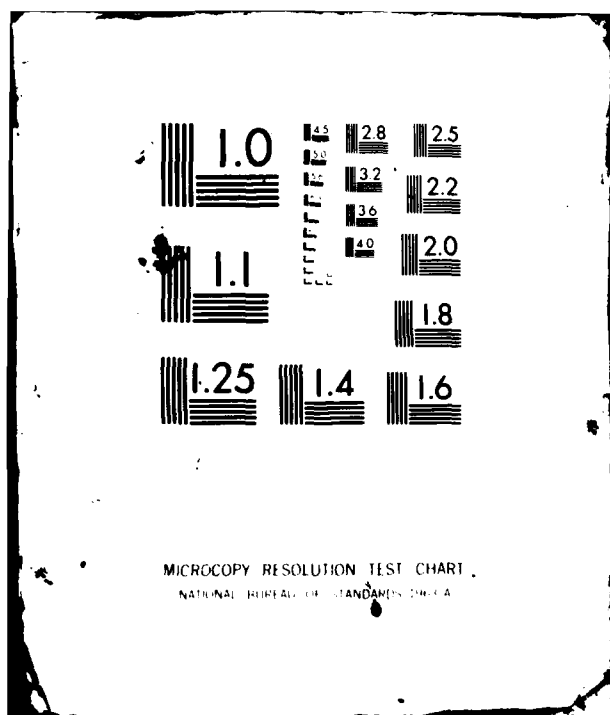
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Technical Summary Report #2289

ON SHAPE NORMALIZATION FOR NON-UNIFORMLY  
ACTIVE CATALYST PELLETS - III

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ON SHAPE NORMALIZATION FOR NON-UNIFORMLY ACTIVE CATALYST PELLETS - III

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ABSTRACT

A new shape normalization for non-uniformly active isothermal catalyst pellets is developed. It is based on the volume average of catalyst activity in a thin reaction zone near the external surface of the active catalyst region, wherein the reaction occurs in the diffusion-controlled regime. This normalization permits inclusion of those catalyst activity profiles that become zero at the external surface of the catalytically active region, which were excluded from previous normalizations. When the surface activity is nonzero, results reduce to those obtained earlier, [1,2]. The normalization provides exactly the slope of the effectiveness factor - Thiele modulus curves, for all pellet shapes and activity profiles, in the limit of diffusion-control. The development is initially made for first-order reactions, and then generalized to include arbitrary reaction rate expressions. Effects of finite external mass transfer resistances are also discussed.

AMS(MOS) Subject Classification - 34B05, 34E05, 80A30

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## SIGNIFICANCE AND EXPLANATION

The effect of diffusion on the rate of chemical reaction in a catalyst pellet is evaluated by the so-called "effectiveness factor," which is the ratio of the actual rate of reaction and that in the absence of transport limitations. For an isothermal first-order reaction, the effectiveness factor is a function of the pellet geometry, the Thiele modulus (which represents how fast the reaction is, relative to diffusion), and the Biot number (which represents the facility of external mass transfer to the pellet, relative to diffusion). If the pellet is uniformly active catalytically, then Aris showed in a classic work [Chem. Eng. Sci., 6, 262 (1957)] that the length dimension used in defining the Thiele modulus and the Biot number could be so redefined, in a physical manner, that the asymptotic behavior of the effectiveness factor for large values of the Thiele modulus (i.e., the diffusion-controlled regime) was identical for various pellet shapes. Fortunately with such a redefinition, the effectiveness factor versus Thiele modulus curves, for the entire range of Thiele modulus values, also virtually coincide for all pellet shapes. Thus, essentially, if one performs computation for one pellet shape, one has simultaneously obtained the effectiveness factor for all pellet shapes.

Now, either as a result of preparation technique, which may well be deliberate, or as a result of use, catalyst pellets develop non-uniform activity profiles. We have recently been attempting [1,2] to provide shape-normalizations in the above sense, when the catalyst activity profile is non-uniform. Various types of activity profiles were previously [1,2] shown amenable to such normalization. The present work brings us one step closer to the eventual goal of including all possible types of activity profiles.

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The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

# ON SHAPE NORMALIZATION FOR NON-UNIFORMLY ACTIVE CATALYST PELLETS - III

M. Morbidelli and A. Varma

## 1. INTRODUCTION

The shape normalization for non-uniformly active catalyst pellets, in which an isothermal first-order reaction occurs, was examined extensively in two previous papers [1,2]. Both the cases of negligible and finite external mass transfer resistance were considered. The particular case of catalyst activity profiles which become zero in a continuous manner somewhere within the pellet or at the pellet external surface, specifically also with negligible external mass transfer resistances, was however previously excluded.

The purpose of the present communication is to develop a physically based shape normalization which also includes this particular situation. In fact, only the asymptotic slope of the effectiveness factor-Thiele modulus curves, for large values of the Thiele modulus (i.e., diffusion-controlled regime), is found amenable to a perfect normalization. The absolute magnitude of the effectiveness factor, even for large values of the Thiele modulus, is found to depend still on parameters that characterize the specific activity profile under consideration. For catalyst activity profiles which do not fit in the category described above, the normalization developed here becomes identical with that given by us earlier [2].

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## 2. ASYMPTOTIC BEHAVIOR AND SHAPE NORMALIZATION

Consider a catalyst pellet with an arbitrary given catalyst activity distribution  $a(x)$ , in which an isothermal first-order reaction occurs with negligible mass transfer resistance external to the active catalyst zone. Let us now examine the behavior of the effectiveness factor for large values of the Thiele modulus.

It is well-known that in the diffusion-controlled regime, the reaction occurs near the surface of the active catalyst zone, within a narrow region whose width is proportional to the reciprocal of the Thiele modulus [3]. This may also be illustrated qualitatively by the following arguments.

The distance,  $\delta$  covered by a diffusing reactant molecule within the pellet can be evaluated from the relationship

$$\delta = (D_e \tau)^{1/2} \quad (1)$$

where  $D_e$  is the effective diffusion coefficient, and  $\tau$  is the characteristic time available to the reactant molecule for diffusing, before it reacts. A reasonable estimate of  $\tau$  can be obtained by considering a batch system, described by the material balance

$$\frac{dC}{dt} = -\bar{k}aC \quad (2)$$

with the initial condition:  $C = C_0$  at  $t = 0$ . In this equation, the catalyst activity  $\bar{a}$  is assumed constant during time. From the solution of eqn (2):

$$C = C_0 \exp(-\bar{k}a\tau), \quad (3)$$

the time-constant for the reaction is

$$\tau = 1/(\bar{k}a). \quad (4)$$

For the diffusion-reaction problem,  $\bar{a}$  would be replaced by  $\bar{a}_\delta$ , the volume average of  $a(x)$  in the active catalyst region where the reaction occurs; substituting this in eqn (1) gives

$$\delta = (D_e / \bar{k} \bar{a}_\delta)^{1/2}. \quad (5)$$

Now, introducing the dimensionless width of the reaction zone  $r_\delta = \delta/R$ , the expected relationship with the Thiele modulus is obtained:

$$r_\delta = \frac{1}{R} \left( \frac{D_e}{\bar{k} \bar{a}_\delta} \right)^{1/2} = \frac{1}{\phi}. \quad (6)$$

Note that  $\bar{a}_\delta$  is the volume average value of the catalyst activity in the reaction zone,  $(R-\delta) \leq x \leq R$ ; i.e.,

$$\bar{a}_\delta = \frac{\int_{R-\delta}^R a(x) dv_p}{\int_{R-\delta}^R dv_p}. \quad (7)$$

The definition of the Thiele modulus, eqn (6), thus obtained is consistent with that used previously [1] for non-uniformly active catalyst pellets; the average value,  $\bar{a}_\delta$  here replaces the surface value,  $a(R)$  employed before.

Introducing the dimensionless space coordinate  $r = x/R$ , and noting from eqn (6) that  $r_\delta \rightarrow 0$  as  $\phi \rightarrow \infty$ , and therefore  $dv_p = S_x dx$  for all pellet shapes, eqn (7) reduces to

$$\bar{a}_\delta = \frac{1}{r_\delta} \int_{1-r_\delta}^1 a(r) dr. \quad (8)$$

The effectiveness factor can be calculated, by definition, as the ratio between the rate of reactant consumption in the actual reaction zone

$(1-r_\delta \leq r \leq 1)$ , and the same quantity in the case of fast diffusion--in which case the reaction occurs within the whole catalytically active region:

$$\eta_a = \frac{(S \delta) (\bar{k} \bar{a}_\delta) C}{V_p (\bar{k} \bar{a}_1) C_s} \quad (9)$$

where the subscript  $a$  denotes the asymptotic value of the effectiveness factor in the diffusion-controlled regime.  $\bar{a}_1$  is, similar to  $\bar{a}_\delta$ , the volume average catalyst activity in the entire catalytically active region (which becomes the reaction zone in the case of fast diffusion; i.e., the kinetic-controlled regime).  $\bar{a}_1$  is therefore given by eqn (7), by replacing  $\delta$  by  $R$ , and this in dimensionless form reduces to

$$\bar{a}_1 = \frac{1}{(n+1)} \int_0^1 a(r) r^n dr. \quad (10)$$

Note that if the catalyst activity profile  $a(x)$  is defined, as done before [1,2], by the ratio between the local rate constant  $k(x)$  and its volume averaged value  $\bar{k}$ , then by definition,  $\bar{a}_1 = 1$  for all pellet shapes and activity profiles. With such activity profiles, the volume average reaction rate constant, in pellets of different shapes and different activity profiles, is the same. Catalyst activity profiles of this type are hereafter called conservative, since they are defined so as to meet the condition of active catalyst conservation.

In eqn (9), the reactant concentration  $C$  in the reaction zone can be estimated as

$$C \approx C_g, \quad (11)$$

since  $r_\delta \rightarrow 0$  as  $\phi \rightarrow \infty$ , and the reaction zone in the limit shrinks to the active catalyst zone surface. With this, eqn (9) gives

$$\eta_a = \frac{S_x \delta}{V_p} \frac{\bar{a}_\delta}{\bar{a}_1}. \quad (12)$$

Also,  $S_x/V_p = (n+1)/R$ , and  $r_\delta = \delta/R$ ; and so

$$\eta_a = (n+1) r_\delta \bar{a}_\delta / \bar{a}_1. \quad (13)$$

If we now introduce a normalized Thiele modulus  $\Phi$ , defined as

$$\Phi = \frac{V_p \bar{a}_1}{S_x \bar{a}_\delta} \left( \frac{\bar{k} \bar{a}_\delta}{D_e} \right)^{1/2} = \frac{\Phi}{n+1} \frac{\bar{a}_1}{\bar{a}_\delta} \quad (14)$$

and substitute eqns (6) and (14) in eqn (13), then

$$\eta_a = 1/\Phi. \quad (15)$$

Thus for different pellet shapes (i.e.,  $n$ ) and for different catalyst activity profiles  $a(x)$ , the asymptotic behavior of  $\eta$  for the diffusion-controlled regime is brought together. Note that for a conservative activity profile (i.e.,  $\bar{a}_1 = 1$ ), the expression of the normalized Thiele modulus given by eqn (14) differs from that used before [1,2] only in that  $\bar{a}_\delta$ , the volume average catalyst activity in the reaction zone, is used in place of the catalyst activity at the outer surface of the catalytically active zone,  $\bar{a}(R)$ .

From eqn (8), it is evident that  $\bar{a}_\delta$  is a function of the reaction zone width,  $r_\delta$  and of the activity profile,  $a(r)$ . Depending on the specific characteristics of the latter, two different possibilities can arise, and these are now identified.

Since we are considering the case of  $\Phi \rightarrow \infty$ , and therefore  $r_\delta \rightarrow 0$ , the activity profile  $a(r)$  may be approximated by its Taylor series around  $r_\delta = 0$  (i.e.,  $r = 1$ ) truncated after the first-order term:

$$a(r) = a(1) + a'(1)r_\delta + O(r_\delta^2) \quad (16)$$

where  $a(1)$  and  $a'(1)$  are the values of catalyst activity and its first derivative, respectively, evaluated at the outer surface of the active catalyst zone (i.e.,  $r = 1$ ). Substituting eqn (16) in eqn (8), and performing the indicated integration gives

$$\bar{a}_\delta = a(1) + a'(1)r_\delta/2 + O(r_\delta^2). \quad (17)$$

If  $a(1) \neq 0$ , then for  $r_\delta \rightarrow 0$  (i.e.,  $\phi \rightarrow \infty$ ),

$$\bar{a}_\delta = a(1). \quad (18)$$

If, however,  $a(1) = 0$ , the limiting value of  $\bar{a}_\delta$ , for  $r_\delta \rightarrow 0$ , becomes a function of  $r_\delta$  and of the derivative of the activity profile,  $a'(1)$ . If the latter quantity is also null, then  $\bar{a}_\delta$  depends on the first nonzero derivative of  $a(r)$  at  $r = 1$ .

The result that we wish to stress here is the following:

- i) if  $a(1) \neq 0$ , then  $\bar{a}_\delta$  is a function only of the activity profile itself;
- ii) if  $a(1) = 0$ , then  $\bar{a}_\delta$  depends also on  $r_\delta$ , and therefore through eqn (6) on the Thiele modulus,  $\phi$ . For this reason, in the relationship between  $\eta_a$  and  $\phi$  given by eqns (14) and (15), the value of  $\bar{a}_\delta$  also affects the asymptotic exponent of the Thiele modulus, and not only the multiplier as in the previous case.

#### 2.1. Case of $a(1) \neq 0$ .

Substituting eqn (18) in (14) gives

$$\phi = \frac{V_p \bar{a}_1}{S_x a(1)} \left( \frac{\bar{k} a(1)}{D_e} \right)^{1/2} \quad (19)$$

which is the same as that obtained before [1,2]. From eqn (15),  $\eta_a = 1/\phi$ . We do not pursue this case further, since it has been examined extensively earlier [1,2].

## 2.2. Case of $a(1) = 0$ .

In this case,  $\bar{a}_\delta$  is a function of  $r_\delta$ , which depends on the specific type of activity profile under consideration. We shall therefore focus on

$$a(r) = m(1-r)^\beta \quad (20)$$

which was examined before [1,2]. Note that for suitable values of  $m$  and  $\beta$ , eqn (20) may be used to approximate many activity profiles which are characterized by  $a(1) = 0$ .

Substituting eqn (20) in eqn (8) gives

$$\bar{a}_\delta = m r_\delta^\beta / (\beta + 1) \quad (21)$$

which using eqn (6) leads to an expression of the reaction zone width:

$$r_\delta = \left( \frac{\beta + 1}{m} \right)^{1/(\beta + 2)} \left( \frac{D_e}{\bar{k}R^2} \right)^{1/(\beta + 2)}. \quad (22)$$

These two equations, together with eqns (14) and (15) give

$$\eta_a = \frac{1}{\bar{\phi}} = \frac{n+1}{\bar{a}_1} \left( \frac{m}{\beta + 1} \right)^{1/(\beta + 2)} \left( \frac{\bar{k}R^2}{D_e} \right)^{-(\beta + 1)/(\beta + 2)} \quad (23)$$

$\bar{a}_1$  may be evaluated from eqn (10) for the specific  $a(r)$  given by eqn (20):

$$\bar{a}_1 = m \frac{(n+1)!}{n+1 \prod_{i=1}^{n+1} (\beta + i)} \quad (24)$$

Finally, introducing  $\phi_0 = R(\bar{k}/D_e)^{1/2}$ , a Thiele modulus based on the average rate constant and the characteristic pellet length, eqn (23) may be rewritten in the form

$$\eta_a = \phi_0^{-2\beta} \frac{(\beta + 1)^{-\beta}}{m^q} \frac{\prod_{i=1}^{n+1} (\beta + i)}{n!} \quad (25)$$

where  $c = 1/(\beta+2)$ ,  $g = (\beta+1)/(\beta+2)$ , and  $n = 0, 2$  indicate the slab and sphere geometries, respectively. Note that  $1/2 < g < 1$ , and so the asymptotic behavior of the effectiveness factor as a function of the Thiele modulus is with an exponent that lies between -1 and -2.

The exact asymptotic expression,  $\eta_e$  obtained from the exact analytic solution (reported in Table 5 of [2]) as  $\phi_0 \rightarrow \infty$  is:

$$\eta_e = \phi_0^{-2g} \frac{(\beta+2)^{\beta c}}{m^g} \frac{\Gamma(q)}{\Gamma(c)} \frac{\prod_{i=1}^{n+1} (\beta+i)}{n!}. \quad (26)$$

A comparison of the two asymptotic expressions, given by eqns (25) and (26), shows that the exponents of the Thiele modulus are identical, but the multipliers are somewhat different. This difference is examined next, but it is first worth noting that eqns (25) and (26) are both valid for arbitrary  $m$  and  $\beta$ , whether they satisfy the conservation condition or not.

### 3. NUMERICAL COMPARISONS

In order to determine the difference between the two asymptotic expressions for  $\eta$ , let us define their ratio

$$\Omega = \eta_e / \eta_a \quad (27)$$

which, using eqns (25) and (26) is given as

$$\Omega = (\beta+1)^c (\beta+2)^{\beta c} \frac{\Gamma(g)}{\Gamma(c)}, \quad (28)$$

a quantity that is a function only of  $\beta$ , and not of pellet shape.

It may now be seen that  $\Omega \rightarrow 1$  as either  $\beta \rightarrow 0$  or  $\beta \rightarrow \infty$ , and so the two asymptotic expressions match in both limits. The value of  $\Omega$  as a function of the activity profile parameter  $\beta$  is shown in Fig. 1. It may be observed that the maximum deviation of  $\eta_a$  from  $\eta_e$  occurs at  $\beta \approx 4.5$ , where the relative percentage error is 14.2%. Moreover,  $\Omega < 1$  for all positive  $\beta$ , which indicates that  $\eta_a$  is an upper bound of the exact asymptote  $\eta_e$ .

A calculation of the effectiveness factor  $\eta$ , in the entire range of the normalized Thiele modulus  $\phi$ , evaluated by using the exact solution (see Table 5 of [2]), is shown in Fig. 2 for the slab ( $n=0$ ) and sphere ( $n=2$ ) geometries, for  $\beta=0$  and 3. As noted above, it may be seen that the asymptotic slopes of the various  $\eta-\phi$  curves for large  $\phi$  are identical, and equal to  $-1$ . The absolute magnitudes of the asymptotes, however, depend on the activity profile parameter  $\beta$ , but not on pellet shape. It may also be observed that the spherical pellet reaches the asymptotic value at relatively larger values of  $\phi$ . This is due to the presence, in the exact asymptotic expression of the effectiveness factor for the sphere (see Table 5 of [2]), of a term proportional to  $\phi_0^{-2}$ , in addition to the leading term proportional to

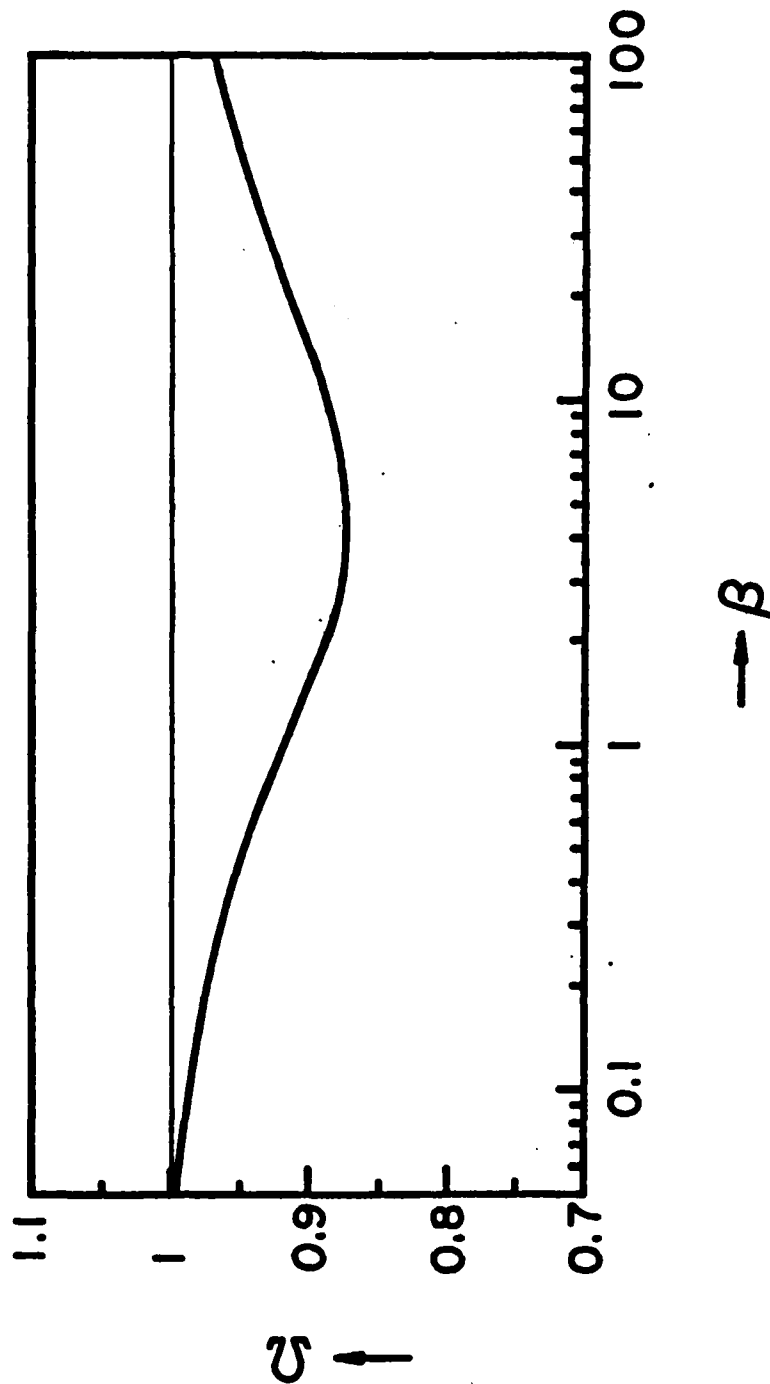


Fig. 1 - The plot of  $\Omega = \eta_e/\eta_a$  vs  $\beta$ , a parameter which characterizes activity profile (20).

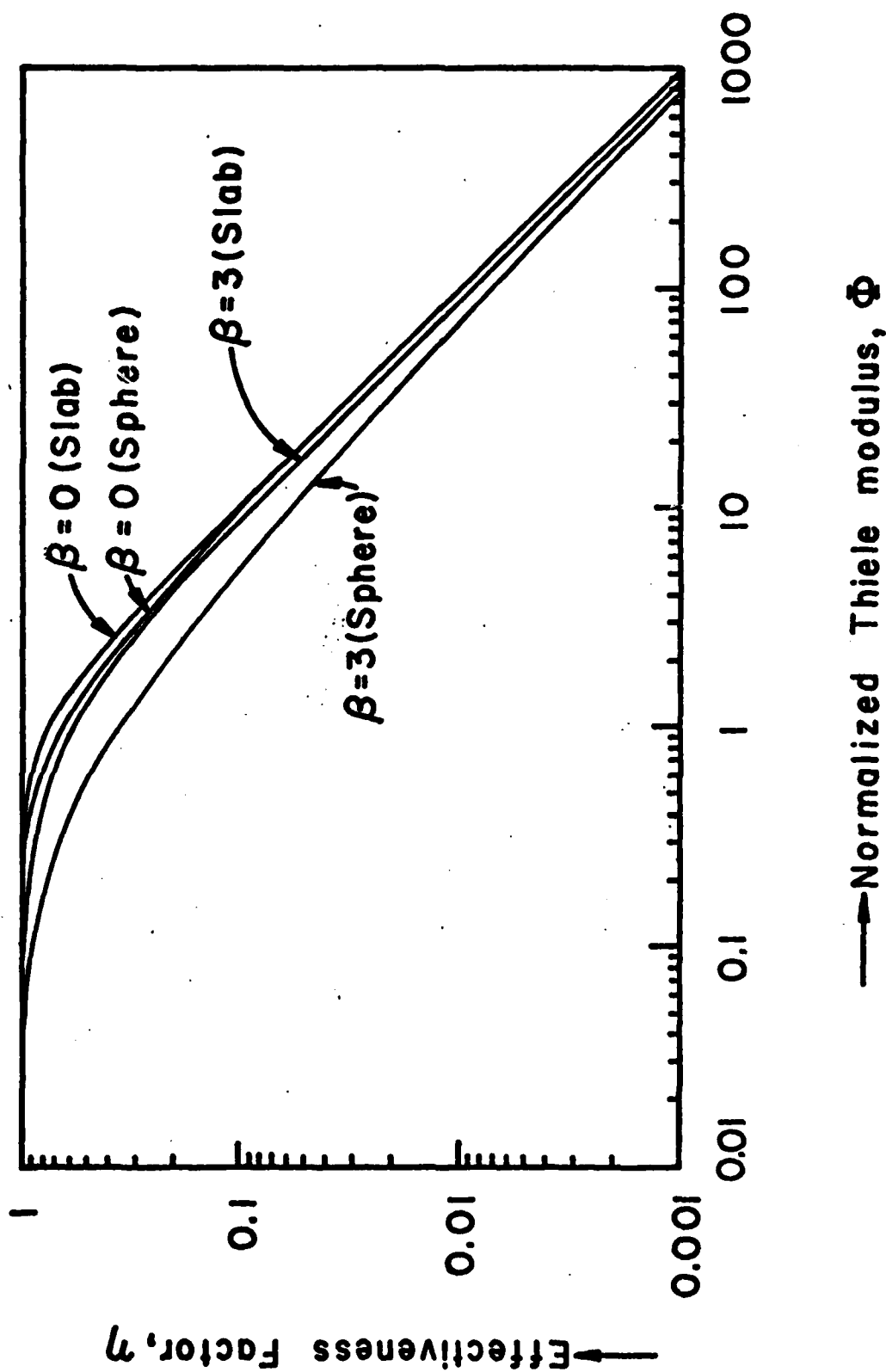


Fig. 2 - Effectiveness factor vs normalized Thiele modulus curves for various pellet shapes and activity profiles (20), with negligible external mass transfer resistances.

$\phi_0^{-2q}$ . Since  $-2 < -2q < -1$ , the term with  $\phi_0^{-2q}$  eventually dominates  $\phi_0^{-2}$ , this feature, however, delays achievement of the asymptotic slope  $-1$ . Note also that this effect becomes more significant at larger values of  $\beta$ .

It is worth reiterating that when  $a(1) = 0$ , the physically based shape normalization developed here, brings only the asymptotic slopes of the effectiveness factor - Thiele modulus curves together for various pellet shapes and activity profiles; the absolute magnitude is not normalized perfectly. A more accurate evaluation of the magnitude of the effectiveness factor would require a more detailed description of the reactant concentration profile close to the outer surface of the active catalyst zone. This means that the reaction time,  $\tau$  would be evaluated through a relationship more accurate than that given by eqn (2), which takes into account both the catalyst activity and the reactant concentration profile in the reaction zone. Such a relationship, however, becomes the same as the starting point of the present diffusion-reaction problem, and so the purpose of an a priori shape normalization is defeated.

#### 4. EFFECT OF EXTERNAL MASS TRANSFER RESISTANCE

Let us now consider a pellet in which the active catalyst is located in an inner core  $0 \leq x < x_2$ , while the balance  $x_2 < x \leq R$  is an inert support. The activity profile thus has the form

$$\begin{cases} a(x) & \text{for } 0 \leq x < x_2 \\ 0 & \text{for } x_2 < x \leq R \end{cases} \quad (29)$$

where  $a(x)$  is an arbitrary given distribution. If external mass transfer resistance in the bulk phase is also taken into account, the problem reduces to the one considered earlier in [2].

It was shown before [2] that the effectiveness factor can be expressed as

$$\eta = \left[ \frac{1}{\eta_D} + \frac{S_2}{S_x} \frac{\phi^2}{\bar{Bi}} + \frac{\phi^2}{\bar{Bi}_{int}} \right]^{-1} \quad (30)$$

where  $\eta_D$  is the effectiveness factor in the case of negligible external mass transfer resistance (i.e., both  $\bar{Bi} = \infty$  and  $\bar{Bi}_{int} = \infty$ ), and whose asymptotic form for large  $\phi$  is given by eqn (15) with  $x_2$  replacing  $R$ . All the other quantities are defined as in [2], simply replacing catalyst activity at the active catalyst zone surface,  $a(1)$  by the average value in the reaction zone,  $\bar{a}_\delta$ . As a consequence, besides the normalized Thiele modulus defined by eqn (14), the normalized pellet characteristic length is also modified, as

$$\bar{R} = V_p / (S_2 \bar{a}_\delta). \quad (31)$$

The variable  $\bar{a}_\delta$  also enters, through eqn (31), definitions of the Biot numbers  $\bar{Bi}$  and  $\bar{Bi}_{int}$ . Note that if  $a(1) \neq 0$ , then due to eqn (18), all these quantities become identical to the corresponding ones in [2].

The effectiveness factor  $\eta$ , can now be represented as a function of its normalized asymptotic value  $\omega$ , derived from eqns (15) and (30) as

$$\omega = \phi + \frac{S_2}{S_x} \frac{\phi^2}{\bar{Bi}} + \frac{\phi^2}{\bar{Bi}_{int}} \quad (32)$$

for all pellet shapes, activity profiles, and external mass transfer resistances,  $\bar{Bi}$  and  $\bar{Bi}_{int}$ . All the  $\eta$ - $\omega$  curves reported in Fig. 2 of [2] are shown in Fig. 3, including also the curves obtained for the activity profile (20) with  $\beta = 0, 0.5, 1, 2$  and  $3$ , for both the slab ( $n=0$ ) and sphere ( $n=2$ ) geometries, and the following set of values for  $\bar{Bi}$  and  $\bar{Bi}_{int}$ :  $5, \infty; \infty, 10; 5, 10$ . The consequent enlargement of the hatched zone is by the lower region in Fig. 3. It may be observed that although the asymptotic behavior, both for small and large  $\phi$ , is identical for all situations, inclusion of activity profile (20) for which  $a(1) = 0$  causes a significant increase in the differences between the various  $\eta$ - $\omega$  curves for intermediate values of  $\omega$ . For example, the width of the hatched region at  $\omega=2$  increases from about 33% to slightly over 60%.

Finally, note that the particular case when both  $\bar{Bi}$  and  $\bar{Bi}_{int}$  are infinite, shown previously in Fig. 2, is excluded in Fig. 3.

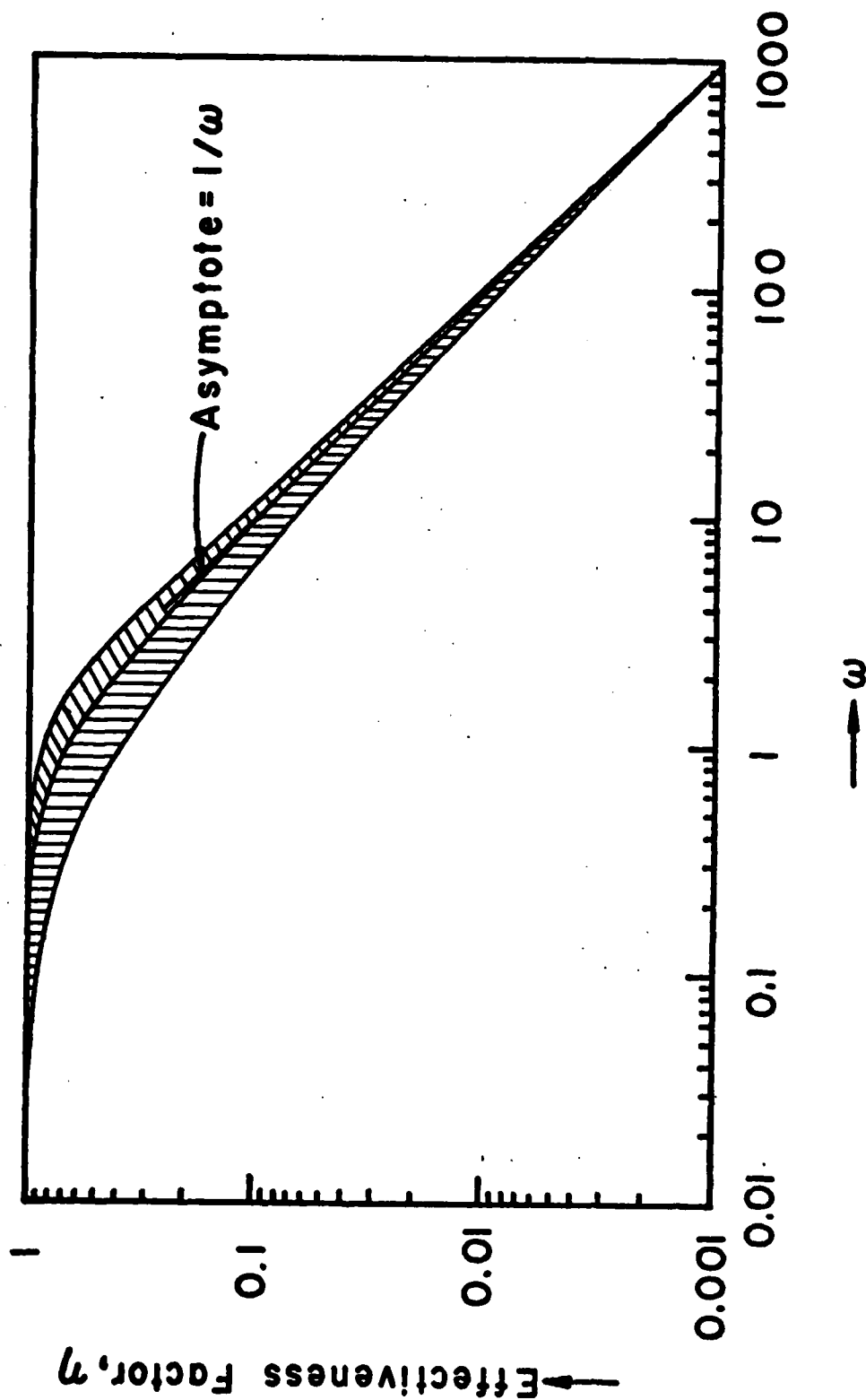


Fig. 3 - Effectiveness factor vs parameter  $\omega$ , defined by eqn (32), for various pellet shapes, activity profiles, and values of external mass transfer resistances.

## 5. EXTENSION FOR ARBITRARY REACTION RATE EXPRESSIONS

The procedure leading to the shape normalization, developed here for first-order reactions, can also be extended to include arbitrary reaction rate expressions, which exhibit positive-order as  $C \rightarrow 0$ . This latter condition is satisfied by all physically reasonable rate expressions, and simply assures that the width of the reaction zone, near the surface of the active catalyst zone, in the diffusion-controlled regime decreases as the Thiele modulus increases; i.e.,  $r_0 \rightarrow 0$  as  $\phi \rightarrow \infty$ .

Consider then a general reaction rate expression  $r(c)$ , the definition of the Thiele modulus modifies, as usual [3], to

$$\phi_0 = R \left[ \frac{r(C_s)}{D_e C_s} \right]^{1/2} \quad (33)$$

while expression (12) for the effectiveness factor does not change, since from eqn (11),  $r(C) \rightarrow r(C_s)$  as  $\phi \rightarrow \infty$ . Following the same steps described above for a first-order reaction, it can again be concluded that  $\eta_a = 1/\phi$  as  $\phi \rightarrow \infty$ .

In terms of the non-normalized Thiele modulus  $\phi_0$ , this implies that the asymptotic slope of the  $\eta$ - $\phi_0$  curve for the catalyst activity profile (20) is again  $-2\alpha$ . This result is indeed confirmed by the numerical computations reported by Villadsen [4], for  $r(C) = \bar{k}C/(1+KC)^2$ . As before, the absolute magnitude of the asymptote of  $\eta$  for large  $\phi_0$  cannot be obtained exactly for this activity profile.

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# NOTATION

$a(x)$	catalyst activity, $k(x)/\bar{k}$
$\bar{a}$	volume average catalyst activity
$Bi$	Biot number, $k_c R/D_e$
$\bar{Bi}$	normalized Biot number, $k_c \bar{R}/D_e$
$\bar{Bi}_{int}$	normalized internal Biot number, $[\int_{y_2}^{y_0} \frac{S_2}{S(y)} dy]^{-1}$
$c$	$1/(\beta+2)$
$C$	reactant concentration
$D$	effective diffusion coefficient
$q$	$(\beta+1)/(\beta+2)$
$k(x)$	local rate constant
$\bar{k}$	volume average rate constant
$k_c$	external mass transfer coefficient
$m$	parameter characterizing activity profile
$n$	integer characteristic of pellet geometry; 0 for infinite slab, 1 for infinite cylinder, 2 for sphere
$r_\delta$	dimensionless width of the reaction zone
$R$	characteristic pellet dimension, half-thickness ( $n=0$ ), radius ( $n=1,2$ )
$\bar{R}$	normalized pellet dimension, $V_p/S_2 \bar{a}_\delta$
$S$	pellet surface area at location $x$
$S_2$	pellet surface area at $x = x_2$
$S_x$	pellet external surface area
$V_p$	pellet volume
$x$	distance from center of pellet; regions $0 \leq x < x_1$ and $x_2 \leq x \leq R$ are inert, while region $x_1 < x < x_2$ is catalytically active.
$y$	normalized distance from center, $x/\bar{R}$
$y_0$	$R/\bar{R}$

### Greek Symbols

$\beta$	parameter characterizing the activity profile
$\delta$	width of the reaction zone
$\Gamma( )$	Gamma function
$\eta$	effectiveness factor
$\eta_D$	effectiveness factor for the Dirichlet problem
$\phi$	Thiele modulus, $R(\bar{k}a_\delta/D_e)^{1/2}$
$\phi_0$	Thiele modulus based on volume average rate constant, $R(\bar{k}/D_e)^{1/2}$
$\phi$	normalized Thiele modulus, defined by eqn (14)
$\tau$	characteristic time for diffusion
$\omega$	parameter defined by eqn (32)
$\Omega$	$\eta_e/\eta_a$

### Subscripts

a	asymptotic value
e	asymptotic value of exact analytic expression
s	surface of catalytically active zone
$\delta$	reaction zone

#### REFERENCES

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20. Abstract (continued)

provides exactly the slope of the effectiveness factor - Thiele modulus curves, for all pellet shapes and activity profiles, in the limit of diffusion-control. The development is initially made for first-order reactions, and then generalized to include arbitrary reaction rate expressions. Effects of finite external mass transfer resistances are also discussed.